PREDICTING ROTATION-VIBRATION LEVELS OF ISOTOPICALLY SUBSTITUTED MOLECULES: WATER AS AN EXAMPLE

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We present the results of prediction of energy levels of various water isotopologues using the fit of mass independent part of potential energy surface (PES) of $H_2{}^{16}O$ only. Fit was done in such a way that mass dependent part of PES - adiabatic correction of $H_2{}^{16}O$ was used during the fit and also non-adiabatic mass-dependent correction to kinetic energy. When the predicted levels of other isotopologues have been calculated, the same mass independent surface as for $H_2{}^{16}O$ was used and both adiabatic and non-adiabatic corrections of the corresponding isotopologues have been employed. As a result the discrepancy between predicted and observed energy levels of $H_2{}^{17}O$ and $H_2{}^{18}O$ were almost of the same value as for $H_2{}^{16}O$ for the levels of $H_2{}^{17}O$ and $H_2{}^{18}O$ known experimentally. It is natural to suppose, that at least for the levels of $H_2{}^{16}O$ included in the fit, the same accuracy of prediction of $H_2{}^{17}O$ and $H_2{}^{18}O$ levels should be expected. Thus, the procedure transferring experimental knowledge of the major isotopologues to the minor isotopologues without the fitting of the levels of these minor isotopologues , has been developed. For other isotopologues such as $D_2{}^{16}O$ and HDO the discrepancy are less perfect, but still within about 0.1 cm^{-1}. These results provide us with a very accurate tool for the prediction of energy levels of minor isotopologues.